JOURNAL OF MOLECULAR STRUCTURE, VOLUME 174 (1988)

AUTHOR INDEX


Acción, F. 83
Adam, M.-Y. 135
Akyüz, S. 435
Alaev, Ju. N. 309
Alix, A. J. P. 159
Amorim da Costa, A. M. 195
Antonović, D. G. 255, 315
Arias, M. S. 273
Arias-Perez, M. S. 267
Aroca, R. 53, 363

Baezold, D. 383
Baezold, M. 383
Baran, E. J. 401
Barańska, H. 417
Barbier, P. 449
Beck, A. 331
Berjot, M. 159
Bleckmann, P. 59
Bogdanović, S. I. 281
Boldeskul, I. E. 297
Breitinger, D. K. 423
Busca, G. 369

Cabello, C. I. 401
Caccinelli, F. 285
Caldeira, M. M. 461
Caminati, W. 285
Carlier, P. 41
Castiglioni, C. 47, 375
Cataliotti, R. S. 285
Cauchetier, M. 369
Cauletti, C. 135
Cavaleiro, A. M. 461
Champarnaud-Mesjard, J.-C. 449
Che Xun 407
Chmurzyński, L. 235
Chotiy, C. Ju. 309
Conesa, J. C. 337
Conflant, P. 449

Dalibart, M. 17
Däufer, H. 11
Davies, J. E. D. 229,435
Day, P. 429
Deiseroth, H.-J. 89
De Lange, C. A. 171
Delwiche, J. 141
Derouault, J. 17
De Saja, J. A. 363
Distefano, G. 177
Dobos, S. 325, 331
Drabe, K. E. 171
Drache, M. 449
Drozdzynski, J. 443
Durig, J. R. 183, 291

Echterhoff, R. 343
Eland, J. H. D. 141
Escolar, D. 83
Eysel, H. H. 35

Fanning, A. R. 183
Fassler, D. 383, 389
Fernandez-Ibañez, M. 267
Fernandez-Sanchez, J.M. 319
Fialkov, Yu. A. 297
Fijala, V. 165
Florencio, F. 273
Förster, H. 357
Franskin-Hubin, M.-J.141
Fritzer, H. P. 429

Gade, R. 389
Galat, V. F. 303,309
Galvez, E. 273
Galvez-Ruano, E. 267
Gatial, A. 207,259
Gatterer, K. 429
Geyer, T. J. 291
Giesbrecht, P. 165
Gil, M. 123
Gil, V. M. S. 461
Ginzburg, A. G. 29
Glasbeek, M. 117
Gooijer, C. 23
Grevels, F.-W. 107
Grimblot, J. 71
Grodzicki, M. 65
Guczi, L. 331
Guerin, R. 95
Guerra, M. 177
Guirgis, G. A. 183
Gussoni, M. 47,375

Hackett, P. A. 113
Hafsi, S. 449
Haller, K. 77
Hanuza, J. 443
Hernandez-Laguna, A. 267
Hofstraat, J. W. 23
Horn, M. 259
Huvenne, J. P. 455

Iriepa, I. 273
Ishikawa, Y. 113
Ito, K. 141
Iza, N.123

Jaaniso, R. 77
Jacke, J. 107
Janowski, A. 201
Jezowska-Trzebiatowska, B. 473
Jodl, H. J. 11
Jones, D. 177
Jordanov, B. 147
Jovanović, B. Ž. 281
Jovanoski, G. 467

Kaden, U. 389
Kalasinsky, V. F. 291
Kamitsos, E. I. 189
Karlsson, A. 207, 215
Kasztelan, S. 71
Kazarian, S. G. 29
Kikas, J. 77
Klaeboe, P. 207, 215, 259
Klotzbücher, W. E. 5
Knott, V. A. 229
Knözinger, E. 89, 343
Koenders, B. G. 171
Kollhoff, H. 89
Koralewski, M. 411
Korte, E. H. 147
Kovacs, G. J. 53
Krstić, V. V. 247, 251
Kühnholz, O. 65

Labarrere, H. 17
Labischinski, H. 165
Lablanquie, P. 141
Lacroix, B. 455
Langel, W. 89
Larsen, R. A. 183
Legendziewicz, J. 473
Lendi, K. 241
Leo, T. J. 83
Le Roy, A. 95
Lewandowski, W. 201, 417
Li Tongxin 407
Lim, K. T. 35
Liwo, A. 235
Lokshin, B. V. 29, 325
Lopez Navarrete, J. T. 375
Lorente, A. 273
Lorenzelli, V. 369
Löwen, W. 11

Maghrawy, H. 473
Mannfors, B. 101
Margulies, L. 153
Martin, F. 363
Mazurak, Z. 443
McDonald, J. K. 291
Modelli, A. 177
Montero, S. 319
Morcillo, J. 123
Muniz-Miranda, M. 351
Murgia, S. M. 285
Murphy, W. F. 319
Mušicatirović, M. D. 247, 251, 281

Nakata, M. 1
Naumann, D. 165
Nenner, I. 141
Neto, N. 351
Nielsen, C. J. 207,215, 259
Nikolić, A. D. 129, 255, 315
Nunziante-Cesaro, S. 325

Oberle, Ch. 35
Paliani, G. 285
Palmö, K. 101
Papavassiliou, G. C. 189
Park, C. G. 1
Payen, E. 71
Pedanou, G. 159
Perišic-Janjić, N. 129
Pešić, M. B. 281
Petrovic, S. D. 129, 255, 315
Piancastelli, M. N. 135
Pietilä, L.-O. 101
Pivovarova, N. S. 297
Plumet, J. 123
Popp, S. 89
Powell, D. L. 259
Prieto, A. C. 363

Quintard, P. 369

Rahhaoui, A. 95
Ramis, G. 369
Ramos, M. L. 461
Ramos, M. N. 47
Rayner, D. M. 113
Remmert, M. 357
Rossini, S. 177
Rybachenko, V. I. 309

Sainz, M. T. 337
Sainz-Diaz, C. I. 267
Santucci, A. 285
Sanz-Aparicio, J. 273
Sbrana, G. 351
Schenkeveld, A. J. 23
Schrader, B. 147
Seevogel, K. 107
Shelyagenko, S. V. 297
Smeyers, Y. G. 267
Smith, J. A. S. 291
Sokołowski, K. 235

Song Guonan 407
Šoptrajanov, B. 467
Soria, J. 337
Sperka, G. 429
Stojanović, N. D. 315
Strek, W. 473
Sülzle, D. 207
Szafranski, M. 411
Szilagyi, T. 395

Tadić, Ž. D. 281
Tarjani, M. 129
Tasumi, M. 1
Terzis, A. 189
Thibud, M. 59
Titov, E. V. 303, 309
Toporowicz, M. 153
Tortajada, J. 83
Tranquille, M. 17
Trippe, H. D. 59
Turrell, G. 41, 455
Turrell, S. 449, 455

Uščumlić, G. S. 247, 251

Valdenebro, A. G. 319
Van Leeuwen, P. A. 117
Velino, B. 285
Velthorst, N. H. 23
Vogt, M. 423

Wawrzynów, A. 235
Wieringa, D. M. 171

Yahia, Z. 455
Yurdakul, S. 435

Zambounis, J. S. 189
Zerbi, G. 47, 375

JOURNAL OF MOLECULAR STRUCTURE, VOLUME 174 (1988)

SUBJECT INDEX

Acylonium salts,
structure and hindered internal rotation in acylonium salts 309
Alkenylphosphonates,
SCF-MO calculations and NMR measurements for alkenyl-phosphonates 267
Amines,
the effects of structure and intermolecular hydrogen bonding on molecular reorientation times of the series of amines and hydrazines 303
Amorphous solids,
statics and dynamics of amorphous solids studied by photoburning of persistent spectral holes (PPSH) 77

Benzene,
spectroscopic investigations of matrix isolated adducts between metal vapors of chromium and benzene 17
Benzene chemisorption,
FTIR study of benzene chemisorption on $Pt/SiO_2$ 395
Benzoic acid,
effect of ionic potentials of metals on perturbation of the aromatic system of benzoic acid 201
Benzoic acids,
comparison of the effect of lanthanides (Ln), d-transition metals and selected metals of the main groups on the aromatic system of salicyclic and benzoic acids 417
Benzyls,
hyperconjugative interactions in benzyls studied by means of ionization energy and electron affinity measurements 177
N-Bicyclo substituted,
synthesis and spectroscopic study of some new rigid N-bicyclo substituted 2-phenylacetamides 255
Bilirubin,
resonance Raman and electronic absorption spectroscopy of bilirubin in solution. An experimental and theoretical study 153
Bromine,
a photoelectron spectroscopic study of molecular chlorine and bromine using three-photon resonant multiphoton ionization 171

Calcium oxide,
uniaxial stress effects on the zero-phonon line emission of the $O_2^-$ defect in calcium oxide 117
Carbon monoxide,
single photon multiionisation of carbon monoxide using synchrotron radiation 141

Carbonyls,
dynamics of metal carbonyls on the infrared time scale: coalescence of CO stretching vibrational bands 107
Carbonyl species,
time-resolved infrared spectroscopy of transient metal carbonyl species in the gas phase 113
Carboxylic acids,
correlation of ultraviolet absorption frequencies of phenyl substituted 2-phenyl-α, β-unsaturated carboxylic acids with Hammett substituent constants 247
$CCl_4$ matrices,
structure and dynamics of solid $CCl_4$ matrices doped with acetonitrile 89
$CF_3$,
torsional transitions and barriers to internal rotation of some molecules with $CF_3$ rotors 183
$\{(\eta\text{-}C_5H_5)Fe(CO)_2\}_2$,
infrared spectra and structure of $\{(\eta\text{-}C_5H_5)Fe(CO)_2\}_2$ adsorbed on oxide surfaces 325
Chlorine,
a photoelectron spectroscopic study of molecular chlorine and bromine using three-photon resonant multiphoton ionisation 171
1-Chloro-4-fluorobut-2-yne,
vibrational spectra and conformations of 1-chloro-4-fluorobut-2-yne 215
3-Chlorothiophene,
the microwave spectrum of 3-chlorothiophene 285
Chromium,
spectroscopic investigations of matrix isolated adducts between metal vapors of chromium and benzene 17
Cinnamic acids,
correlation of ultraviolet absorption frequencies of cis and trans substituted cinnamic acids with Hammett substituent constants 251
Cluster compounds,
characterization of the "surface enhanced Raman scattering" by use of Raman-spectroscopic and quantum mechanical investigations of simple cluster compounds 59
CO stretching,
dynamics of metal carbonyls on the infrared time scale: coalescence of CO stretching vibrational bands 107
$Cs_2NaYCl_6$,
absorption and luminescence spectra of $U^{3+}$ in $Cs_2NaYCl_6$ 443
Cyclohexyl azide,
the IR and Raman spectra and conformations of cyclohexyl azide 207

Decomposing overlapping bands,
a comparison of methods for decomposing overlapping bands in Raman spectra 101
Diazines,
SER spectra of diazines adsorbed on silver sols: spectroscopic evidence of reduction products 351
1,3-Dibromo-2,2-dimethylpropane,
vibrational spectra and conformations of 1,3-bromo-2,2-dimethylpropane (DBDMP) and 2,2-di(fluoromethyl)-1,3-difluoropropane (TFN) 259

Dichlorocyclopentylphenyl tertiary phosphine complexes,
the low frequency vibrational spectra of some dichlorocyclopentylphenyl tertiary phosphine complexes of palladium(II) and platinum(II) 407
Differential FTIR spectroscopy,
differential FTIR spectroscopy with polarized radiation 147
2,2-Di(fluoromethyl)-1,3-difluoropropane,
vibrational spectra and conformations of 1,3-dibromo-2,2-dimethylpropane (DBDMP) and 2,2-di(fluoromethyl)-1,3-difluoropropane (TFN) 259
Dilute solutions,
on the infrared absorption profiles of dilute solutions 41

Ethanes,
torsional transitions in the conventional Raman spectrum of ethanes 319
N-Ethylacetamide,
hydrogen bonding of N-monosubstituted amides. IR study of N-ethylacetamide and N-methylpropionamide 129

Formamide,
molecular aggregation of ionic surfactants in formamide studied by laser Raman spectroscopy 195
Four-level systems,
general dynamics of four-level systems including relaxation 241

n-Hexane,
temperature dependent site structure of the phenalenyl radical in n-pentane and n-hexane Shpol'skii matrices 23
Hydrazines,
the effects of structure and intermolecular hydrogen bonding on molecular reorientation times of the series of amines and hydrazines 303
9-(2'-Hydroxyethyl)-9-azabicyclo{3.3.1}nonan-3α-ol,
synthesis and structural study of 9-(2'-hydroxyethyl)-9-azabicyclo{3.3.1} nonan-3α-ol 273

Inclusion compounds,
clathrate and inclusion compounds. Part 10. Solid state $^{13}C$ NMR studies of inclusion compounds 229
Intensity parameters,
comparison of experimental and "ab initio" intensity parameters 47
Ionic surfactants,
molecular aggregation of ionic surfactants in formamide studied by laser Raman spectroscopy 195
IR,
IR study of hydrogen bonds formed by π-complexes of transition metals in liquid xenon solution 29

β-Lactam derivatives,
amide resonance and FT-IR spectra of some β-lactam derivatives: application of resolution enhancement procedures in Fourier space 123
Lanthanide perchlorates,
spectroscopic properties of lanthanide perchlorates in nonaqueous solutions 473

Magnesium oxide,
FT-IR characterization of adsorption complexes on magnesium oxide surfaces 343
4-Methoxybenzylidene-4'-butyl-aniline (MBBA) fluorinated analogues,
conformational analysis of 4-methoxybenzylidene-4'butylaniline (MBBA) fluorinated analogues by $^{1}H$ and $^{13}C$ - NMR 297
N-Methyl-N-cycloalkyl substituted,
configurations in unsymmetrically N-methyl-N-cycloalkyl substituted 2-phenylacetamides 315
N-Methylpropionamide,
hydrogen bonding of N-mono-substituted amides. IR study of N-ethylacetamide and N-methyl-propionamide 129

$N_2$/rare-gas mixed crystals,
Raman studies on $N_2$/rare-gas mixed crystals 11
Neodymium(III) azide,
spectroscopic studies and crystal field investigations on a complex neodymium(III) azide 429
Ni(110) surface,
theoretical investigation of adsorption of water dimers on a Ni(110) surface 65

Organic conductors,
resonance Raman studies in the organic conductors α- and β-(PEDT-TTF)$_3$I$_3$ and β-(DMPEDT-TTF)$_3$I$_3$ 189

Oxo-anions,
Raman intensities and polarizability parameters (EOPs) of some oxo-anions of Group V, VI and VII elements in aqueous solution: general trends 35
Oxygen radical,
quantum chemical assessment of the structure of an oxygen radical adsorbed on titania and detected by ESR spectroscopy 337

Pathogenic bacteria,
the rapid differentiation and identification of pathogenic bacteria using Fourier transform infrared spectroscopic and multivariate statistical analysis 165
n-Pentane,
temperature dependent site structure of the phenalenyl radical in n-pentane and n-hexane Shpol'skii matrices 23
$PH_3$,
photoionization of the outer- and inner-valence shells of $PH_3$ in the photon energy range 30-90 eV 135
2-Phenylacetamides,
configurations in unsymmetrically N-methyl-N-cycloalkyl substituted 2-phenylacetamides 315
synthesis and spectroscopic study of some new rigid N-bicyclo substituted 2-phenylacetamides 255
Photoburning,
statics and dynamics of amorphous solids studied by photoburning of persistent spectral holes (PPSH) 77
Platinum(II),
tuning of the trans-influence in sulfito-complexes of platinum(II) 423

Polyacetylene,
interpretation of vibrational spectra of pristine, doped and photoinduced polyacetylene 375
Polymethine dyes,
energy and electron transfer processes of adsorbed polymethine dyes 383
PPSH ,
statics and dynamics of amorphous solids studied by photoburning of persistent spectral holes (PPSH) 77
1,2-Propanediol,
infrared-induced conformational isomerization and reverse reaction in the dark of 1,2-propanediol in low-temperature argon matrices 1
Proteins,
fast determination of the quantitative secondary structure of proteins by using some parameters of the Raman amide I band 159
Purine,
structure and equilibria of purine in ethanol. An UV study 83
$PV_{14}O_{42}^{9-}$ polyanion,
vibrational and electronic spectra of the $PV_{14}O_{42}^{9-}$ polyanion 401
Pyridine N-oxides,
experimental studies on the UV-spectra of substituted pyridine N-oxides and their perchlorates in acetonitrile 235
Pyrrole polymerization,
SERS study of the pyrrole polymerization 363

Quinoline complexes,
an infrared and Raman spectroscopic study of transition metal(II) halide quinoline complexes 435

$Re_2(CO)_{10}$,
FTIR study of interaction of $Re_2(CO)_{10}$ with silica and alumina supports 331
Reflectance spectra,
quantitative evaluation of reflectance spectra of light-scattering media 389
Rhenium,
rhenium carbonyl and dinitrogen complexes: identification of intermediates by matrix isolation photochemistry and metal atom synthesis 5

Saccharinates,
bonding of the carbonyl group in metal saccharinates: correlation with the infrared spectra 467
Salicylic acids,
comparison of the effect of lanthanides (Ln), d-transition metals and selected metals of the main groups on the aromatic system of salicylic and benzoic acids 417
Scandium hexafluorides,
vibrational spectra, phase transitions and force-fields in crystalline scandium hexafluorides 449

Semiconducting hexaborides,
Raman and FTIR investigations of metallic and semiconducting hexaborides 455
Silicon carbide,
FT-IR characterization of Si-H bonds on the surface of silicon carbide 369
Silver-coated,
surface enhanced Raman scattering on silver-coated tin spheres 53
Silver sols,
SER spectra of diazines adsorbed on silver sols: spectroscopic evidence of reduction products 351
5-Substituted-3-isopropyl-6-methyl uracils,
$^1H$ NMR spectra of some 5-substituted-3-isopropyl-6-methyl uracils 281
Sulfito-complexes,
tuning of the trans-influence in sulfito-complexes of platinum(II) 423

Tartaric acid salts,
absorption of some tartaric acid salts and their aqueous solutions 411
Tin spheres,
surface enhanced Raman scattering on silver-coated tin spheres 53
Titania,
quantum chemical assessment of the structure of an oxygen radical adsorbed on titania and detected by ESR spectroscopy 337
Transition metals,
IR study of hydrogen bonds formed by π-complexes of transition metals in liquid xenon solution 29
sym-Triazine,
infrared band structures at the phase transition in sym-triazine 95

$U^{3+}$,
absorption and luminescence spectra of $U^{3+}$ in $Cs_2NaYCl_6$ 443

Vanadium(V) complexation,
multinuclear NMR study of vanadium(V) complexation with tartaric and citric acids 461
Vinylsilane,
vibrational-rotational analysis of some of the fundamentals of vinylsilane 291

Water dimers,
theoretical investigation of adsorption of water dimers on a Ni(110) surface 65
$WO_3(MoO_3)/\gamma Al_2O_3$ catalysts,
in situ laser Raman spectroscopy of the sulphiding of $WO_3(MoO_3)/\gamma Al_2O_3$ catalysts 71

Xenon solution,
IR study of hydrogen bonds formed by π-complexes of transition metals in liquid xenon solution 29

Zeolites A,
infrared studies on the interaction of $N_2O$ adsorbed in transition metal ion-exchanged zeolites A 357

CONTENTS OF VOLUME 174

(The second of three Congress Volumes)

Infrared-induced conformational isomerization and reverse reaction in the dark of 1,2-propanediol in low-temperature argon matrices
C. G. Park, M. Nakata and M. Tasumi (Tokyo, Japan) ..... 1

Rhenium carbonyl and dinitrogen complexes: identification of intermediates by matrix isolation photochemistry and metal atom synthesis
W. E. Klotzbücher (Mülheim a.d. Ruhr, F.R.G.) ..... 5

Raman studies on $N_2$/rare-gas mixed crystals
H. Däufer, W. Lowen and H. J. Jodl (Kaiserslautern, F.R.G.) ..... 11

Spectroscopic investigations of matrix isolated adducts between metal vapors of chromium and benzene
M. Dalibart, J. Derouault, H. Labarrere and M. Tranquille (Talence, France) ..... 17

Temperature dependent site structure of the phenalenyl radical in n-pentane and n-hexane Shpol'skii matrices
J. W. Hofstraat, A. J. Schenkeveld, C. Gooijer and N. H. Velthorst (Amsterdam, The Netherlands) ..... 23

IR study of hydrogen bonds formed by $\pi$-complexes of transition metals in liquid xenon solution
B. V. Lokshin, S. G. Kazarian, A. G. Ginzburg (Moscow, U.S.S.R.) ..... 29

Raman intensities and polarizability parameters (EOPs) of some oxo-anions of Group V, VI and VII elements in aqueous solution: general trends
H. H. Eysel, K. T. Lim and Ch. Oberle (Heidelberg, F.R.G.) ..... 35

On the infrared absorption profiles of dilute solutions
P. Carlier and G. Turrell (Villeneuve, France) ..... 41

Comparison of experimental and "ab initio" intensity parameters
M. Gussoni (Genova, Italy and Milano, Italy), M. N. Ramos (UFPE, Brasil and Milano, Italy), C. Castiglioni and G. Zerbi (Milano, Italy) ..... 47

Surface enhanced Raman scattering on silver-coated tin spheres
R. Aroca (Windsor, Ont., Canada) and G. J. Kovacs (Mississauga, Ont., Canada) ..... 53

Characterization of the 'Surface Enhanced Raman Scattering' by use of Raman-spectroscopic and quantum mechanical investigations of simple cluster compounds
P. Bleckmann, M. Thibud and H. D. Trippe (Dortmund, F.R.G.) ..... 59

Theoretical investigation of adsorption of water dimers on a Ni(110) surface
M. Grodzicki and O. Kühnholz (Hamburg, F.R.G.) ..... 65

In situ laser Raman spectroscopy of the sulphiding of $WO_3(MoO_3)/\gamma Al_2O_3$ catalysts
E. Payen (Lasir, C.N.R.S.), S. Kasztelan and J. Grimblot (Villeneuve, France) ..... 71

Statics and dynamics of amorphous solids studied by photoburning of persistent spectral holes (PPSH)
J. Kikas, K. Haller and R. Jaaniso (Tartu, U.S.S.R.) ..... 77

Structure and equilibria of purine in ethanol. An UV study
F. Acción, D. Escolar, J. Tortajada (Puerto Real, Spain) and T. J. Leo (Madrid,Spain) ..... 83

Structure and dynamics of solid $CCl_4$ matrices doped with acetonitrile
H.-J. Deiseroth, S. Popp, H. Kollhoff, W. Langel and E. Knözinger (Siegen, F.R.G.) ..... 89

Infrared band structures at the phase transition in sym-triazine
A. L. Roy, A. Rahhaoui and R. Guerin (Poitiers, France) ..... 95

A comparison of methods for decomposing overlapping bands in Raman spectra
K. Palmö, B. Mannfors and L.-O. Pietilä (Helsinki, Finland)
..... 101

Dynamics of metal carbonyls on the infrared time scale: coalescence of CO stretching vibrational bands
F.-W. Grevels, J. Jacke and K. Seevogel (Mülheim a.d. Ruhr, F.R.G.)
..... 107

Time-resolved infrared spectroscopy of transient metal carbonyl species in the gas phase
Y. Ishikawa, P. A. Hackett and D. M. Rayner (Ottawa, Ont., Canada)
..... 113

Uniaxial stress effects on the zero-phonon line emission of the $O_2^-$ defect in calcium oxide
P. A. van Leeuwen and M. Glasbeek (Amsterdam, The Netherlands)
..... 117

Amide resonance and FT-IR spectra of some β-lactam derivatives: application of resolution enhancement procedures in Fourier space
M. Gil, J. Plumet, N. Iza and J. Morcillo (Madrid, Spain) ..... 123

Hydrogen bonding of N-monosubstituted amides. IR study of N-ethylacetamide and N-methylpropionamide
A. D. Nikolić, M. Tarjani, N. Perišić-Janjić (Novi Sad, Yugoslavia) and S. D. Petrović (Belgrade, Yugoslavia) ..... 129

Photoionization of the outer- and inner-valence shells of $PH_3$ in the photon energy range 30-90 eV
C. Cauletti, M. N. Piancastelli (Rome, Italy) and M.-Y. Adam (Orsay, France) ..... 135

Single photon multiionisation of carbon monoxide using synchroton radiation
P. Lablanquie (Orsay, France), J. Delwiche, M.-J. Franskin-Hubin (Liege, Belgium), I. Nenner (Gif-sur-Yvette, France), J. H. D. Eland (Oxford, Gt. Britain) and K. Ito (Ibaraki-ken, Japan) ..... 141

Differential FTIR spectroscopy with polarized radiation
B. Jordanov (Sofia, Bulgaria), E. H. Korte (Dortmund, F.R.G.) and B. Schrader (Essen, F.R.G.) ..... 147

Resonance Raman and electronic absorption spectroscopy of bilirubin in solution. An experimental and theoretical study
L. Margulies and M. Toporowicz (Rehovot, Israel) ..... 153

Fast determination of the quantitative secondary structure of proteins by using some parameters of the Raman amide I band
A. J. P. Alix, G. Pedanou and M. Berjot (Reims, France) ..... 159

The rapid differentiation and identification of pathogenic bacteria using Fourier transform infrared spectroscopic and multivariate statistical analysis
D. Naumann, V. Fijala, H. Labischinski and P. Giesbrecht (Berlin, Germany) ..... 165

A photoelectron spectroscopic study of molecular chlorine and bromine using three-photon resonant multiphoton ionisation
B. G. Koenders, D. M. Wieringa, K. E. Drabe and C. A. de Lange (Amsterdam, The Netherlands) ..... 171

Hyperconjugative interactions in benzyls studied by means of ionization energy and electron affinity measurements
G. Distefano (Ferrara, Italy), A. Modelli, M. Guerra, D. Jones and S. Rossini (Bologna, Italy) ..... 177

Torsional transitions and barriers to internal rotation of some molecules with $CF_3$ rotors
J. R. Durig, R. A. Larsen (Columbia, SC, U.S.A.), G. A. Guirgis and A. R. Fanning (Charleston, SC, U.S.A.) ..... 183

Resonance Raman studies in the organic conductors α- and β- (PEDT--TTF)$_3$I$_3$ and β-(DMPEDT-TTF)$_3$I$_3$
J. S. Zambounis, E. I. Kamitsos, G. C. Papavassiliou and A. Terzis (Athens, Greece) ..... 189

Molecular aggregation of ionic surfactants in formamide studied by laser Raman spectroscopy
A. M. Amorim da Costa (Coimbra, Portugal) ..... 195

Effect of ionic potentials of metals on perturbation of the aromatic system of benzoic acid
W. Lewandowski and A. Janowski (Warsaw, Poland) ..... 201

The IR and Raman spectra and conformations of cyclohexyl azide
D. Sülzle, A. Gatial, A. Karlsson, P. Klaeboe and C. J. Nielsen (Oslo, Norway) ..... 207

Vibrational spectra and conformations of 1-chloro-4-fluorobut-2-yne
A. Karlsson, P. Klaeboe and C. J. Nielsen (Oslo, Norway) ..... 215

Spectroscopic study of some condensed piperidine bicyclanols
E. Galvez, M. S. Arias, I. Ardid, J. Bellanato and J.V. Garcia-Ramos (Madrid, Spain) ..... 223

Clathrate and inclusion compounds. Part 10. Solid state $^{13}$C NMR studies of inclusion compounds
J. E. D. Davies and V. A. Knott (Lancaster, Gt. Britain) ..... 229

Experimental studies on the UV-spectra of substituted pyridine N-oxides and their perchlorates in acetonitrile
A. Wawrzynów, K. Sokolowski, L. Chmurzyński and A. Liwo (Gdansk, Poland) ..... 235

General dynamics of four-level systems including relaxation
K. Lendi (Zurich, Switzerland) ..... 241

Correlation of ultraviolet absorption frequences of phenyl substituted 2-phenyl-α , β-unsaturated carboxylic acids with Hammett substituent constants
V. V. Krstić, G. S. Ušćumlić and M. D. Muškatirović (Beograd, Yugoslavia) ..... 247

Correlation of ultraviolet absorption frequences of cis and trans substituted cinnamic acids with Hammett substituent constants
G. S. Uščumlić, V. V. Krstić and M. D. Muškatirović (Beograd, Yugoslavia) ..... 251

Synthesis and spectroscopic study of some new rigid N-bicyclo substituted 2-phenylacetamides
D. G. Antonović, S. D. Petrović (Belgrade, Yugoslavia) and A. D. Nikolić (Novi Sad, Yugoslavia) ..... 255

Vibrational spectra and conformations of 1,3-dibromo-2,2-dimethyl-propane (DBDMP) and 2,2-di(fluoromethyl)-1,3-difluoropropane (TFN)
A. Gatial, M. Horn, P. Klaeboe, C. J. Nielsen and D. L. Powell (Oslo, Norway) ..... 259

SCF-MO Calculations and NMR measurements for alkenylphosphonates
Y. G. Smeyers, A. Hernandez-Laguna, M. Fernandez-Ibañez, C. I. Sainz-Diaz, E. Galvez-Ruano and M. S. Arias-Perez (Madrid, Spain) ..... 267

Synthesis and structural study of 9-(2'-hydroxyethyl)-9-azabicyclo[3.3.1]-nonan-3α-ol
I. Iriepa, A. Lorente, M. S. Arias, E. Galvez, F. Florencio, J. Sanz-Aparicio (Madrid, Spain) ..... 273

$^{1}H$ NMR Spectra of some 5-substituted-3-isopropyl-6-methyl uracils
B. Z. Jovanović, Z. D. Tadić, M. D. Muskatirović, M. B. Pešić and S. I. Bogdanović (Belgrade, Yugoslavia) ..... 281

The microwave spectrum of 3-chlorothiophene
W. Caminati, B. Velino (Bologna, Italy), F. Caccinelli, R. S. Cataliotti, S. M. Murgia, G. Paliani and A. Santucci (Perugia, Italy) ..... 285

Vibrational-rotational analysis of some of the fundamentals of vinyl-silane
J. K. McDonald (Redstone Arsenal, AL, U.S.A.), V. F. Kalasinsky, J. A. S. Smith (MS, U.S.A.), T. J. Geyer and J. R. Durig (Columbia, SC, U.S.A.) ..... 291

Conformational analysis of MBBA fluorinated analogues by $^{1}H$ and $^{13}C$ - NMR
N. S. Pivovarova, I. E. Boldeskul, S. V. Shelyagenko and Yu.A. Fialkov (Kiev, U.S.S.R.) ..... 297

The effects of structure and intermolecular hydrogen bonding on molecular reorientation times of the series of amines and hydrazines
V. F. Galat and E. V. Titov (Donetsk, U.S.S.R.) ..... 303

Structure and hindered internal rotation in acylonium salts
E. V. Titov, V. I. Rybachenko, V. F. Galat, C.Ju. Chotiy and Yu. N. Alaev (Donetsk, U.S.S.R.) ..... 309

Configurations in unsymmetrically N-methyl-N-cycloalkyl substituted 2-phenylacetamides
S. D. Petrović, N. D. Stojanović, D. G. Antonović (Belgrade, Yugoslavia) and A. D. Nikolić (Novi Sad, Yugoslavia) ..... 315

Torsional transitions in the conventional Raman spectrum of ethanes
J. M. Fernandez-Sanchez, A. G. Valdenebro, S. Montero and W. F. Murphy (Madrid, Spain) ..... 319

Infrared spectra and structure of $[(\eta\text{-}C_5H_5)Fe(CO)_2]_2$ adsorbed on oxide surfaces
S. Dobos (Budapest, Hungary), S. Nunziante-Cesaro (Rome, Italy) and B. V. Lokshin (Moscow, U.S.S.R.) ..... 325

FTIR Study of interaction of $Re_2(CO)_{10}$ with silica and alumina supports
S. Dobos, A. Beck and L. Guczi (Budapest, Hungary) ..... 331

Quantum chemical assessment of the structure of an oxygen radical adsorbed on titania and detected by ESR spectroscopy
J. C. Conesa, M. T. Sainz and J. Soria (Madrid, Spain) ..... 337

FT-IR Characterization of adsorption complexes on magnesium oxide surfaces
R. Echterhoff and E. Knözinger (Siegen, F.R.G.) ..... 343

SER Spectra of diazines adsorbed on silver sols: spectroscopic evidence of reduction products
M. Muniz-Miranda, G. Sbrana (Firenze, Italy) and N. Neto (Potenza, Italy) ..... 351

Infrared studies on the interaction of $N_2O$ adsorbed in transition metal ion-exchanged zeolites A
H. Förster and M. Remmert (Hamburg, F.R.G.) ..... 357

SERS Study of the pyrrole polymerization
F. Martin, A. C. Prieto, J. A. de Saja (Valladolid, Spain) and R. Aroca (Windsor, Ont., Canada) ..... 363

FT-IR Characterization of Si-H bonds on the surface of silicon carbide
P. Quintard, G. Ramis (Limoges, France), M. Cauchetier (Gif-sur-Yvette, France), G. Busca and V. Lorenzelli (Genova, Italy) ..... 369

Interpretation of vibrational spectra of pristine, doped and photoinduced polyacetylene
C. Castiglioni, G. Zerbi (Milano, Italy), J. T. L. Navarrete (Milano, Italy and Malaga, Spain) and M. Gussoni (Genova, Italy) ..... 375

Energy and electron transfer processes of adsorbed polymethine dyes
D. Fassler, M. Baezold and D. Baezold (Jena, G.D.R.)..... 383

Quantitative evaluation of reflectance spectra of light-scattering media
D. Fassler, R. Gade and U. Kaden (Jena, G.D.R.) ..... 389

FTIR Study of benzene chemisorption on $Pt/SiO_2$
T. Szilagyi (Budapest, Hungary) ..... 395

Vibrational and electronic spectra of the $PV_{14}O_{42}^{9-}$ polyanion
E. J. Baran and C. I. Cabello (La Plata, Argentina) ..... 401

The low frequency vibrational spectra of some dichlorocyclopentylphenyl tertiary phosphine complexes of palladium(II) and platinum(II)
Che Xun, Song Guonan and Li Tongxin (Dalian, P.R. China) ..... 407

Absorption of some tartaric acid salts and their aqueous solutions
M. Koralewski and M. Szafranski (Poznan, Poland) ..... 411

Comparison of the effect of lanthanides (Ln), d-transition metals and selected metals of the main groups on the aromatic system of salicylic and benzoic acids
W. Lewandowski and H. Barańska (Warsaw, Poland) ..... 417

Tuning of the trans-influence in sulfito-complexes of platinum(II)
D. K. Breitinger and M. Vogt (Erlangen, F.R.G.) ..... 423

Spectroscopic studies and crystal field investigations on a complex neodymium(III) azide
K. Gatterer, H. P. Fritzer, G. Sperka (Graz, Austria) and P. Day (Oxford, Gt. Britain) ..... 429

An infrared and Raman spectroscopic study of transition metal(II) halide quinoline complexes
S. Yurdakul (Ankara, Turkey), S. Akyüz (Samsum, Turkey) and J. E. D. Davies (Lancaster, Gt. Britain) ..... 435

Absorption and luminescence spectra of $U^{3+}$ in $Cs_2NaYCl_6$
Z. Mazurak, J. Hanuza and J. Drozdzynski (Wroclaw, Poland) ..... 443

Vibrational spectra, phase transitions and force-fields in crystalline scandium hexafluorides
S. Turrell, S. Hafsi, P. Conflant, P. Barbier, M. Drache (Villeneuve, France) and J.-C. Champarnaud-Mesjard (Limoges, France) ..... 449

Raman and FTIR investigations of metallic and semiconducting hexaborides
S. Turrell, Z. Yahia, G. Turrell (Villeneuve, France), J. P. Huvenne and B. Lacroix (Lille, France) ..... 455

Multinuclear NMR study of vanadium(V) complexation with tartaric and citric acids
M. Madalena Caldeira, V. M. S. Gil (Coimbra, Portugal), M. L. Ramos and A. M. Cavaleiro (Aveiro, Portugal) ..... 461

Bonding of the carbonyl group in metal saccharinates: correlation with the infrared spectra
G. Jovanovski and B. Šoptrajanov (Skopje, Yugoslavia) ..... 467

Spectroscopic properties of lanthanide perchlorates in nonaqueous solutions
J. Legendziewicz, B. Jeżowska-Trzebiatowska, W. Stręk (Wroclaw, Poland) and H. Maghrawy (Cairo, Egypt) ..... 473

Author index ..... 477

Subject index ..... 480